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Dirichlet Inversion and Lattice Inversion Problem

YUCHUAN WEI, GUANGWEN YAN AND QISHAN ZHANG
Department of Electrical Engineering, No. 202
Beijing University of Aeronautics and Astronautics
Beijing, 100083, P.R. China
yuchuanwei@21cn.com

KAI YAO
Department of Physics, Xinxiang Senior Teachers College
Xinxiang, Henan, 453000, P.R. China

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Abstract—Another application of Dirichlet multiplication is considered in this note. We show that Dirichlet inversion in number theory plays an important role in lattice inversion problem. With the help of this concept, lattice inversion problem becomes straightforward. © 2001 Elsevier Science Ltd. All rights reserved.

1. INTRODUCTION

In our recent papers, such as [1,2], the application of Dirichlet multiplication to electronics was considered carefully. In this note, its application to solid state physics is discussed.

Lattice inversion problem is to determine the pairwise potential (v) from cohesive energy (V) which can be *ab initio* calculated or experimentally measured [3–8]. Suppose that λ is a Bravais lattice (see [9,10]) with an identical atom at every lattice point. We can represent the cohesive energy per atom as a sum of pairwise potential

$$V = \frac{1}{2} \sum_{\mathbf{r} \in \lambda \setminus \{\mathbf{0}\}} v(|\mathbf{r}|). \tag{1}$$

Conversely, the lattice inversion problem in solid state physics asks how to represent pairwise potential v by means of the cohesive energy V in case the cohesive energy is obtained from experiment or theory.

The one-dimensional lattice inversion problem is trivial. By means of Theorem 270 in [11], from

$$V(x) = v(x) + v(2x) + v(3x) + \cdots + v(nx) + \cdots, \tag{2}$$

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it follows directly that [4]

$$v(x) = V(x) - V(2x) - V(3x) - \cdots + \mu(n)V(nx) + \cdots, \tag{3}$$

where μ denotes the moebius function [12]. In this letter, x always denotes lattice constant.

We shall show that Dirichlet inversion in number theory [12] plays an important role in the multidimensional lattice inversion problem.

First, let us introduce a formula related to Dirichlet inversion.

FORMULA. *$c(n)$ is an arithmetical function and $c^{-1}(n)$ is its Dirichlet inversion. We have*

$$F(t) = \sum_{n=1}^{\infty} c(n) f\left(\sqrt{n}\,t\right) \Longleftrightarrow f(t) = \sum_{n=1}^{\infty} c^{-1}(n) F\left(\sqrt{n}\,t\right). \tag{4}$$

PROOF. In fact, we have

$$\begin{aligned}
\sum_{n=1}^{\infty} c^{-1}(n) F\left(\sqrt{n}\,t\right) &= \sum_{n=1}^{\infty} c^{-1}(n) \sum_{m=1}^{\infty} c(m) f\left(\sqrt{mn}\,t\right) \\
&= \sum_{k=1}^{\infty} \sum_{n|k} c^{-1}(n) c\left(\frac{k}{n}\right) f\left(\sqrt{k}\,t\right) \\
&= \sum_{k=1}^{\infty} \delta_{k1} f\left(\sqrt{k}\,t\right) \\
&= f(t)
\end{aligned}$$

and vice versa.

With this formula, multidimensional lattice inversion problem will become easy and simple.

2. TWO-DIMENSIONAL LATTICES

(a) Square lattice [9,10].

The cohesive energy $V(x)$ and pairwise potential $v(x)$ are related by

$$V(x) = \frac{1}{2} \sum_{n=1}^{\infty} r_2(n) v\left(\sqrt{n}\,x\right), \tag{5}$$

$$v(x) = 2 \sum_{n=1}^{\infty} r_2^{-1}(n) V\left(\sqrt{n}\,x\right). \tag{6}$$

Here, $r_2(n)$ denotes the number of atoms whose distance from the fixed atom is $\sqrt{n}\,x$. In other words, $r_2(n)$ is the number of integer solutions of the equation [9]

$$\xi_1^2 + \xi_2^2 = n. \tag{7}$$

Its explicit expression is [11,13]

$$r_2(n) = 4 \sum_{d|n} \chi_1(d) = 4\chi_1 * e(n), \tag{8}$$

where * denotes Dirichlet multiplication [12], and χ_1 and e are defined by

$$\chi_1(n) = \begin{cases} 1, & n = 4l+1, \\ 0, & n = 4l+2, \\ -1, & n = 4l+3, \\ 0, & n = 4l+4, \end{cases} \qquad (l = 0, 1, 2, 3, \dots), \tag{9}$$

and

$$e(n) = 1 \qquad \text{for } n = 1, 2, 3, \dots. \tag{10}$$

Consequently, the inverse function $r_2^{-1}(n)$ can be expressed as

$$r_2^{-1} = \frac{1}{4}\chi_1^{-1} * e^{-1} = \frac{1}{4}\mu\chi_1 * \mu \tag{11}$$

or

$$r_2^{-1}(n) = \frac{1}{4}\sum_{d|n} \mu(d)\chi_1(d)\mu\left(\frac{n}{d}\right). \tag{12}$$

(b) Hexagonal lattice [9,10].

The cohesive energy $V(x)$ and pairwise potential $v(x)$ are related by

$$V(x) = \frac{1}{2}\sum_{n=1}^{\infty} h(n)v\left(\sqrt{n}\,x\right), \tag{13}$$

$$v(x) = 2\sum_{n=1}^{\infty} h^{-1}(n)V\left(\sqrt{n}\,x\right). \tag{14}$$

Here $h(n)$ denotes the number of atoms whose distance from the fixed atom is $\sqrt{n}\,x$. In other words, $h(n)$ is the number of integer solutions of the equation [9]

$$\xi_1^2 + \xi_1\xi_2 + \xi_2^2 = n. \tag{15}$$

Its explicit expression is [13]

$$h(n) = 6\sum_{d|n} \chi_2(d) = 6\chi_2 * e(n), \tag{16}$$

where χ_2 are defined by

$$\chi_2(n) = \begin{cases} 1, & n = 3l+1, \\ -1, & n = 3l+2, \\ 0, & n = 3l+3, \end{cases} \qquad (l = 0, 1, 2, 3, \dots). \tag{17}$$

Similarly, the inverse function $h^{-1}(n)$ can be expressed as

$$h^{-1} = \frac{1}{6}\chi_2^{-1} * e^{-1} = \frac{1}{6}\mu\chi_2 * \mu \tag{18}$$

or

$$h^{-1}(n) = \frac{1}{6}\sum_{d|n} \mu(d)\chi_2(d)\mu\left(\frac{n}{d}\right). \tag{19}$$

REMARK. Without Dirichlet inversion, it would be very difficult to solve the inversion problems of these two lattices (see [6]).

3. THREE-DIMENSIONAL LATTICES

(a) Simple cubic (sc) lattice. The cohesive energy $V(x)$ and pairwise potential $v(x)$ are related by

$$V(x) = \frac{1}{2}\sum_{n=1}^{\infty} r_3(n)v\left(\sqrt{n}\,x\right), \tag{20}$$

$$v(x) = 2\sum_{n=1}^{\infty} r_3^{-1}(n)V\left(\sqrt{n}\,x\right). \tag{21}$$

Similarly, $r_3(n)$ denotes the number of atoms whose distance from the fixed atom is $\sqrt{n}\,x$. In other words, $r_3(n)$ is an arithmetical function defined as the number of integer solutions of the equation

$$\xi_1^2 + \xi_2^2 + \xi_3^2 = n. \tag{22}$$

By the equation

$$\sum_{n=0}^{\infty} r_3(n) q^n = \left(1 + 2q + 2q^4 + 2q^9 + 2q^{16} + \cdots + 2q^{m^2} + \cdots\right)^3, \tag{23}$$

one can efficiently calculate the first finite values of $r_3(n)$ [9]. In order to calculate its values associated to very large n, or study its behavior as $n \to \infty$, please use its explicit formula in [13, Section 8.9].

(b) Face-centered cubic (fcc) lattice

The cohesive energy $V(x)$ and pairwise potential $v(x)$ are related by

$$V(x) = \frac{1}{2} \sum_{n=1}^{\infty} r_{\mathrm{fcc}}(n) v\left(\sqrt{n}\,\frac{x}{2}\right) \tag{24}$$

$$= \frac{1}{2} \sum_{k=1}^{\infty} r_3(2k) v\left(\sqrt{2k}\,\frac{x}{2}\right) \tag{25}$$

$$= \frac{1}{2} \sum_{n=1}^{\infty} r_3'(n) v\left(\frac{1}{2}\sqrt{2n}\,x\right), \tag{26}$$

$$v(x) = 2 \sum_{n=1}^{\infty} r_3'^{-1}(n) V\left(\sqrt{2n}\,x\right). \tag{27}$$

In equation (24), $r_{\mathrm{fcc}}(n)$ denotes the number of atoms whose distance from the fixed atom is $\sqrt{n}\,(x/2)$. From the structure of the fcc lattice [9], it follows that $r_{\mathrm{fcc}}(n)$ is the number of integer solutions of the equation system

$$\begin{aligned} &\xi_1^2 + \xi_2^2 + \xi_3^2 = n, \\ &\xi_1 + \xi_2 + \xi_3 \equiv 0, \qquad (\mathrm{mod}\, 2). \end{aligned}$$

Since

$$\xi_1^2 \equiv \xi_1, \quad \xi_2^2 \equiv \xi_2, \quad \xi_3^2 \equiv \xi_3, \qquad (\mathrm{mod}\, 2),$$

we have

$$\xi_1 + \xi_2 + \xi_3 \equiv \xi_1^2 + \xi_2^2 + \xi_3^2, \qquad (\mathrm{mod}\, 2).$$

Furthermore, we have

$$r_{\mathrm{fcc}}(n) = \begin{cases} 0, & n = 1, 3, 5, \ldots, \\ r_3(n), & n = 2, 4, 6, \ldots. \end{cases} \tag{28}$$

In the resultant equations (25) and (26), the arithmetical function $r'(n)$ is defined by

$$r_3'(n) = r_3(2n),$$

and $r_3'^{-1}(n)$ is its Dirichlet inverse.

REMARK. The inversion coefficients by Chen in [7] is none other than the first few values of r_3^{-1} and $r_3'^{-1}$. The Dirichlet inversion makes the meaning of inversion coefficient clear. What is more, by properties of Dirichlet inversion, one can study the behavior of r_3^{-1} and $r_3'^{-1}$ at very large ns so that the convergent speed and error of the inversion algorithm can be considered. This is a necessary step to unify the discrete atom model and continuous medium model for crystals.

APPENDIX

Table 1. A short table of the functions used in this letter.

n	1	2	3	4	5	6	7	8	9	10	$\cdots$
$e(n)$	1	1	1	1	1	1	1	1	1	1	$\cdots$
$\mu(n)$	1	-1	-1	0	-1	1	-1	0	0	1	$\cdots$
$\chi_1(n)$	1	0	-1	0	1	0	-1	0	1	0	$\cdots$
$\chi_2(n)$	1	-1	0	1	-1	0	1	-1	0	1	$\cdots$
$r_2(n)$	4	4	0	4	8	0	0	4	4	8	$\cdots$
$r_2^{-1}(n)$	$\frac{1}{4}$	$-\frac{1}{4}$	0	0	$-\frac{1}{2}$	0	0	0	$-\frac{1}{4}$	$\frac{1}{2}$	$\cdots$
$h(n)$	6	0	6	6	0	0	12	0	6	0	$\cdots$
$h^{-1}(n)$	$\frac{1}{6}$	0	$-\frac{1}{6}$	$-\frac{1}{6}$	0	0	$-\frac{1}{3}$	0	0	0	$\cdots$
$r_3(n)$	6	12	8	6	24	24	0	12	30	24	$\cdots$
$r_3^{-1}(n)$	$\frac{1}{6}$	$-\frac{1}{12}$	$-\frac{2}{9}$	0	$-\frac{2}{3}$	$-\frac{1}{9}$	0	$-\frac{1}{4}$	$-\frac{29}{54}$	1	$\cdots$
$r_{\mathrm{fcc}}(n)$	0	12	0	6	0	24	0	12	0	24	$\cdots$
$r'_3(n)$	12	6	24	12	24	8	48	6	36	24	$\cdots$
$r_3'^{-1}(n)$	$\frac{1}{12}$	$-\frac{1}{24}$	$-\frac{1}{6}$	$-\frac{1}{16}$	$-\frac{1}{6}$	$\frac{1}{9}$	$-\frac{1}{3}$	$\frac{1}{32}$	$\frac{1}{12}$	0	$\cdots$

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